Numerical analysis of optimum packing structure of particles on a spherical surface

***Takuya Uehara[1]**

[1]Department of Mechanical Systems Engineering, Yamagata University, Japan.

*Presenting author: uehara@yz.yamagata-u.ac.jp

Abstract

Numerical analyses on the particle-packing structures on a spherical surface are performed. The particles are assumed to have uniform radius and connected by inter-particle interaction. The positions of the particles are justified to minimize the interaction energy, which is assumed to be represented by two-body potential function. The number of particles N and radius ratio x of the particles to the central large sphere are varied as the model parameters. As a result, it revealed that filling all the space by the hexagonal packing on a sphere surface is impossible and some defects are needed. Also the optimized arrangement of the defects presents a regular pattern. In conclusion, the availability of the present method for the optimization of the particle packing structure is fairly validated.

Keywords: Particle packing, Optimization problem, Close packed structure, Molecular dynamics method, Computer simulation.

Introduction

Advanced materials using nano- or micro-particles have been developed and applied for various engineering fields such as electronics, biological and medical engineering, and so on. The packing structure of particles plays an important role on the functionality of the material, and the arrangement of the particles is one of the most definitive factors in the material design. In general, to set the particles artificially on designed sites is difficult, and hence self-organization process is often utilized. In such processes, however, the structure obtained is limited, and more suitable structures may exist to generate much higher performance. Therefore, we have been investigating the optimum structures of particle packing for specified purposes. Considering when arranging particles with uniform radius on a planar face, for instance, it is well known that the densest packing is achieved when the centers of particles are disposed on the regular triangular positions making regular hexagonal arrangement, which is often referred to as honeycomb arrangement. Concerning the three-dimensional structures, the closest packed structure is well known as the face-centered cubic (fcc) or hexagonal close packed (hcp) structures, which is achieved by accumulating this hexagonal plane to the perpendicular direction.

This kind of simple problem is, however, very complicated if the applied condition is varied; for instance, when the shape of particles is not sphere, when the size of particles are not identical, and when the particles are arranged on a curved surface. Since the analytical solutions for these problems are difficult to obtain, we have been approaching them using numerical analysis [1][2]. Particularly, in this study, the packing structures of small spherical particles with uniform radius on a spherical surface with relatively large radius are investigated, and the optimum structures are discussed on the basis of relation between the number of particles and the radius of the surface.

Simulation model and conditions

In this study, completely spherical particles with uniform radius r are considered. These particles are adhered on a convex surface of a sphere of radius R. The particles are assumed to

have interaction to the other particles with strong repulsion and weak attraction, and also elastic attraction on the spherical surface. The optimum arrangement of the particles is numerically searched by moving the particles. This procedure is similar to that of molecular dynamics method, and hence the algorithm is employed. The interaction between two particles are represented by Lennard-Jones type potential function, $\phi = 4\varepsilon((\sigma/r)^{12}-(\sigma/r)^{6})$, and linear spring connection with the sphere surface is assumed. The interacting forces between particles and the elastic force from the central sphere are calculated, and every particle is moved depending on the force vector. The interacting force is relaxed as repeating the motion, and finally stable arrangement is expected to be obtained.

The initial positions of particles are randomly provided, while the center of the large sphere on which particles are adhered is set as the origin of the coordinate system. Standardized dimension is employed so that the particle diameter r = 1.0, and the radius R of the large sphere are varied. L-J parameters are taken as σ = 0.893 and ε = 0.002, where the value in σ is taken as the equilibrium inter-particle distance to be 1.0. The elastic force on the surface is assumed to be $F = k\ (d - d_0)$ where d is the distance from the center of the large sphere, and $d_0 = r + R$ (see Fig. 1).

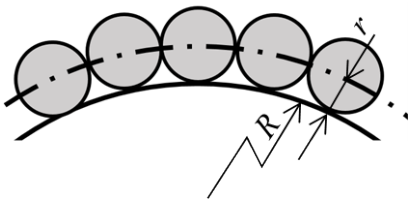


Figure 1. Particles on a large sphere surface.

Total number of particles, N, to be put on the surface is varied. Theoretical maximum number is defined for a planar problem as follows. The area of the unit hexagon in Fig. 2 is calculated as $S_{hex} = (6/\sqrt{3})\ r^2 \approx 3.46\ r^2$, and hence the maximum number of particle can be calculated as S/S_{hex}, while some influence of the considering domain area should be taken into account especially when S is relatively small. Anyway, in the spherical case, the area of the surface is represented as $S = 4\pi(R+r)^2$, and hence the optimum number of particles is derived as

$$N_{opt} = 4\pi(R+r)^2 / (\sqrt{3}\ r^2) = 3.63\ ((R+r)/r)^2 . \qquad (1)$$

In the present model, r = 1.0 and hence it is represented as

$$N_{opt} = 3.63\ (R+1)^2. \qquad (2)$$

When the number of particle N is given, on the other hand, the optimum radius R_{opt} is provided as

$$R_{opt} = (0.275\ N)^{1/2} - 1. \qquad (3)$$

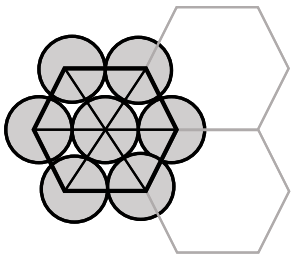


Figure 2. Hexagonal close packed structure.

These values indicate the ideal structure under hexagonal packing, but it is impossible to achieve on the spherical surface due to the effect of curvature and periodicity. Additionally, soft-core particle is assumed instead of hard sphere, and hence these values are used only as a referential one.

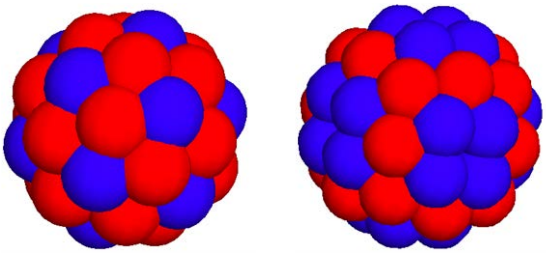
From a different viewpoint, geometric feature of regular polyhedron is helpful for predicting the particle packing structure on the spherical surface. Regular polyhedron consists of regular polygonal planes, and the surface of a sphere can be approximated to be consisting of these planes. Then the particle packing manner is similar to those in the planar problem, i.e. honeycomb arrangement on each polygon. In this context, it is not necessarily regular polyhedron, but semi-regular polyhedron consisting of two or more types of polyhedra is regarded. This procedure is not complete because the irregularity on the edges and vertexes are unavoidable, but the similarity will be worth noting.

Total number of particles N and the radius R of the sphere on which the particles are adhered are employed as the simulation parameters. The particle radius r is kept constant to be $r = 1.0$ for all cases. The simulations are carried out for a given radius R with various numbers of particles N. The initial positions of particles are set randomly, and hence several trials are demonstrated. The optimum configuration of particles are selected from all data for the given R and presented in the following sections.

Results and discussion − Case 1: relatively large particles

Firstly, the results for the cases when the radius R is relatively small, i.e. the particle radius is relatively large, are shown in this section. Figure 3 (a) shows the particle arrangement for R = 2.0 obtained by N = 32. Color indicates the number of particles in the nearest-neighbor distance, n_d, which is 6 for ideal hexagonal arrangement. In Fig. 3, blue and red represents n_d = 5 and 6, respectively. The particles are arranged regularly; every red particle is connected by three red particles and three blue ones, and every blue particle is surrounded by five red ones. The predicted optimum number for this radius is calculated as N_{opt} = 32.7 from Eq. (2), and actually the result shows the optimum structure for this radius. If taking these particles on the center of certain polyhedra, the red and blue particles are corresponding to regular hexagons and pentagons, respectively; i.e. the sphere corresponds to be approximated by a truncated icosahedron, and the number of particles N = 32 is identical to the number of plane of the truncated icosahedron. This structure is similar to that observed as fullerene C60 or well known as soccer ball pattern.

Figure 3 (b) shows the result for R = 2.5, for which N_{opt} = 44.5, and a regular pattern is observed when N = 44. The blue particles (n_d = 5) are assembled together making square arrangement, and red particles (n_d = 6) surround the squared four blue particles. Also the number of square assembly is 6, and they are disposed in the orthogonal orientation, like the Cartesian x, y and z axes. This structure seems on the basis of a cube; four particles in each 6 square face, one on each 8 vertex, and one on each 12 edge of the cube.



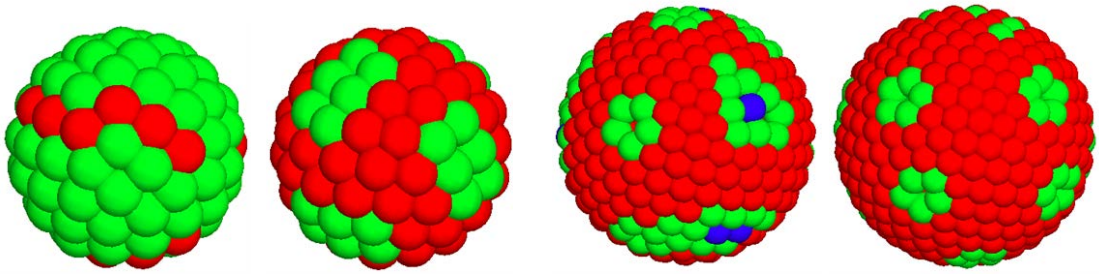
(a) R = 2.0, N = 32 (b) R = 2.5, N = 44

Figure 3. Simulation results obtained for relatively large particles.

In this way, the optimum packing structure is observed on regular polyhedron or some other regular pattern, when the relative particle radius is large.

Results and discussion − Case 2: relatively small particles

Next, in this section, the results for the case when the particle radius is relatively small and many particles are adhered on the sphere surface. Both Figs. 4 (a) shows the result for R = 4.0, for which N_{opt} = 90.8, and Figs. (i) and (ii) show the result for N = 90 and 100, respectively. In these figures, blue, green, and red particles represent n_d = 4, 5, and 6, respectively. Generally, as the number of particles becomes larger, it becomes more difficult to explore the completely optimum structure. Nevertheless, candidate structures can be found. In Fig. 4 (a)(i) for N = 90, most particles have 5 neighbors (n_d = 5), and regularity in the arrangement cannot be observed. The value of 5 in n_d indicates less density than the ideal packing, and more particles should be adhered on the surface. Then the result for N = 100 shows better results with more number of ideal density. The regularity of the particles are not perfect but it shows similar tendency to that in Fig. 3(b); six particles of n_d = 5 depicted in green color assembled together making rectangular shape, and each assembly is surrounded by red particles.

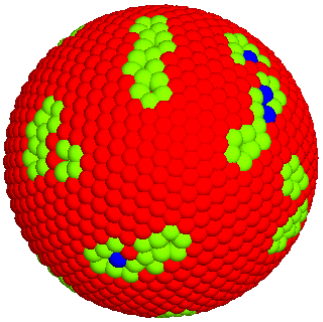


(i) N = 90 (ii) N = 100 (i) N = 294 (ii) N = 325

(a) R = 4.0 (b) R = 8.0

Figure 4. Simulation results obtained for relatively small particles.

For the case of R = 8.0 (N_{opt} = 294.0), the result for N = 294 is shown in Fig. 4(b)(i). A few particles have only four neighbors, and some vacant spaces are also observed, while the ratio of the particles of n_d = 6 is higher than that shown in Fig. 4(a)(i). This feature implies that the formation of local defects tends to be unavoidable. In this case, the better regularity was found for N = 325, as shown in Fig. 4(b)(ii). Many particles have 6 neighbors, and some particles with 5 neighbors are scattered. Characteristic feature in this case is that the particles surrounding the vacancy form pentagonal assembly of particles with n_d = 5, and the vacancy sites are regularly dispersed.



R = 16.0, N = 1120

Figure 5. Simulation results for very small particles.

As the radius of the particles becomes much smaller and the number of particles gets larger, it becomes more difficult to obtain the complete regularity and resultant optimum structure. For example, Figure 5 represents the result for R = 16.0 (N_{opt} = 1049.1) by N = 1120. Several vacancy and pentagonal arrangement can be observed, but the regularity in their arrangement was not clarified so far, and further analysis will be reported in the near future.

Conclusions

In this paper, numerical scheme for analyzing the optimum structure when small particles are adhered on a spherical surface was presented. A simple model with inter-particle interaction and adhesion with a simple elastic connection was assumed, and the effectivity was shown. In the case that the particle radius is relatively small, regular pattern was obtained. The geometrical similarity to the polyhedral structure was also found. When the particle radius is relatively small and number of particles is large, then it was difficult to find absolutely optimum structure, but it revealed that several specific local structures are formed. As a conclusion, the method presented in this paper is effective for exploring the optimum particle packing structures, and further analysis is to be continued.

References

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